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(NASA-TH-89774) ON A NEW FORM OF ADIABATIC PERTURBATION THEORY IN THE PROBLEM OF PARTICLE INTERACTION WITH A QUANTUM FIELD (NASA) 26 p

On a New Form of Adiabatic Perturbation Theory in the
Problem of Particle Interaction with a Quantum Field

Ukrainskii Matematicheskii Zhurnal, vol. 2, No. 2, 1950 pp. 3 - 24

The Hamiltonian usually analyzed in investigating particle motion in a quantum field is:

$$H = H_p + H_v + H_{int}$$

in which H_p corresponds to the particle intrinsic energy, H_v to the quantum field energy, H_{int} to the energy of particle-field interaction.

In order to deal with a discrete spectrum, the whole system is considered in a certain finite space of volume V, for example, in a cube with side $L = \sqrt{V}$, and nonperiodic boundary conditions are imposed. Here, it is understood that the passage to the limit as $V \to \infty$, corresponding to the transition to a continuous spectrum, is always kept in mind.

If the analyzed quantum field can be expanded into noninteracting oscillators, then:

$$H_{\mathbf{v}} = \frac{1}{2} \sum_{(\mathbf{f})} h \omega_{\mathbf{f}} (b_{\mathbf{f}} \dot{b}_{\mathbf{f}} + \dot{b}_{\mathbf{f}} b_{\mathbf{f}})$$

where $\omega_{\mathbf{f}}$ is the oscillator frequency; $\mathbf{b}_{\mathbf{f}}$, $\dot{\mathbf{b}}_{\mathbf{f}}$ are the quantum amplitudes with known commutation relations corresponding to Bose statistics. The $\dot{\mathbf{f}}$ generate a discrete spectrum for finite V which transforms into a continuous one as $V \to \infty$. Thus, for example, $\dot{\mathbf{f}}$, in many problems, is the quasi-wave vector with the components $\left(\frac{2\pi}{L} \, \mathbf{n}_1, \frac{2\pi}{L} \, \mathbf{n}_2, \frac{2\pi}{L} \, \mathbf{n}_3\right)$, where $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ are positive and negative integers.

For nonrelativistic particles without an external field:

$$H_{p} = \frac{p^2}{2\mu} = -\frac{h^2}{2\mu} \Delta_{p}$$

The same expression can be used when an external field exists, if only the method of equivalent mass is used.

A typical form of the interaction energy is the expression of the three-dimensional, homogeneous field linearly dependent on the quantized functions, for example:

$$H_{int} = \int K(\vec{r} - \vec{r}') \psi(\vec{r}') d\vec{r}' + \int K(\vec{r} - \vec{r}') \psi(\vec{r}') d\vec{r}'$$

Expanding $\psi(\vec{r})$ in plane waves normalized in the volume V:

$$\psi(\mathbf{r}) = \sum_{(\mathbf{f})} \mathbf{b}_{\mathbf{f}} \frac{\mathbf{e}^{\mathbf{i}(\mathbf{f}\mathbf{r})}}{\sqrt{\mathbf{V}}}$$

we arrive at the expression:

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$$H_{\text{int}} = \sum_{(f)} \left\{ 2L_f e^{i(\hat{f}r)} b_f + 2\hat{L}_f e^{-i(\hat{f}r)} b_f \right\}$$

in which the \mathfrak{A}_{f} , \mathfrak{A}_{f}^{*} are proportional to $\frac{1}{\sqrt{V}}$.

In this paper, we used the cited typical expressions for $_{p}^{H}$, $_{v}^{H}$, $_{int}^{H}$ and, therefore, we assume that:

(1)
$$H = \frac{\overline{p}^{2}}{2\mu} + \frac{1}{2} \sum_{(f)}^{\infty} h\omega_{f}(b_{f}b_{f} + b_{f}b_{f}) + \sum_{(f)}^{\infty} \left\{ U_{f}e^{i(\widehat{f}r)}b_{f} + \mathring{\mathcal{J}}_{f}e^{-i(\widehat{f}r)}b_{f} \right\}$$

Hamiltonians of this form are considered in various problems.

Let us recall the problems of impurity-particle motion in helium II [1,2,3]; electron motion in a semiconductor [4], nucleon interaction with a scalar meson field in the nonrelativistic approximation.

Somewhat more complex Hamiltonians, but of substantially the same form, are analyzed also in nonrelativistic theories of electron interaction with an electromagnetic field, of nucleon interaction with pseudoscalar and vector meson fields, etc.

Let us note that although the analyzed Hamiltonian (1) is one of the simplest

in the problems of particle interaction with a quantum field, the exact solution of the appropriate wave equation is impossible in every case in the modern state of the science.

Consequently, approximate methods of perturbation theory must be drawn upon.

The known, ordinary schemes of this theory are used directly in analyzing the case of weak coupling of particles with a field when the principal terms in the Hamiltonian are $H_{\mathbf{p}}$ and $H_{\mathbf{p}}$ and $H_{\mathbf{p}}$ is a small perturbation.

However, in a number of problems the particle-field coupling cannot be considered weak.

For example, let us indicate the case of strong coupling when H_{int} is proportional not to a small but to a large parameter and also the, mathematically-similar, case of 'adiabatic coupling' when the field 'kinetic energy' is small.

Let us take a specific example and let us analyze just the motion of an electron in an ionic crystal using the model proposed by S. I. Pekar [4].

In this model the existence of the periodic field of the ionic lattice is taken into account by the effective mass method and, consequently, it is considered that

$$H_p = \frac{1}{2\mu}^2$$

The electron interaction with the lattice is considered as specified by its interaction with the polarizing (optical) waves corresponding to inertial polarization. Here, the ionic lattice itself is replaced by a dielectric continuum.

Starting from these representations, H int is taken as:

$$H_{int} = -e \int \frac{\left(\overrightarrow{P}(\overrightarrow{r})(\overrightarrow{r} - \overrightarrow{r}) \right)}{\left| \overrightarrow{r} - \overrightarrow{r} \right|^3} d\overrightarrow{r}$$

where $\overrightarrow{P(r)}$ is a vector corresponding to the inertial part of the specific polarization.

Since H_{int} is not zero only for longitudinal waves, the transverse waves can be eliminated from the considerations completely and the field of longitudinal waves can be taken as the quantum field with which the electron interacts.

Then, expanding $\overrightarrow{P}(\overrightarrow{r})$ in plane waves normalized over the volume V, we can write:

$$\vec{P}(\vec{r}) = \sum_{(f)} \frac{\vec{f}}{|\vec{f}|} P_f \frac{e^{i(fr)}}{\sqrt{V}} ; P_f = P_{-f}$$

and P_f can be considered as the generalized complex coordinates characterizing the field.

Using this expansion, we obtain:

$$H_{int} = 4\pi e \sum_{(f)} \frac{1}{|f| \sqrt{V}} P_f e^{i(fr)}$$

Finally, the field energy in the Pekar theory is:

$$H_{\mathbf{v}} = \frac{1}{2} \sum_{(\mathbf{f})} \frac{\mu_{\mathbf{f}}}{c_{\mathbf{f}}} (P_{\mathbf{f}} P_{-\mathbf{f}} + P_{\mathbf{f}} P_{-\mathbf{f}}) = \frac{1}{2} \sum_{(\mathbf{f})} \left\{ \frac{\mu_{\mathbf{f}}}{c_{\mathbf{f}}} P_{\mathbf{f}} P_{-\mathbf{f}} - \frac{h^2 \omega_{\mathbf{f}}^2 c_{\mathbf{f}}}{\mu_{\mathbf{f}}} \frac{\partial^2}{\partial P_{\mathbf{f}} \partial P_{-\mathbf{f}}} \right\}$$

where $\omega_{\hat{\mathbf{f}}}$ are the frequencies of the ion optical oscillations; $\mathbf{c}_{\hat{\mathbf{f}}}$ are certain constants.

Therefore, the complete Hamiltonian describing the motion of the electron in the ionic crystal in the model considered is represented by the expression:

(2)
$$H = -\frac{h^2}{2\mu} \Delta_{\mathbf{r}} + 4\pi e \sum_{(\mathbf{f})} \frac{1}{|\mathbf{f}|} \mathbf{p}_{\mathbf{f}} e^{\mathbf{i}(\mathbf{f}\mathbf{r})} + \frac{1}{2} \sum_{(\mathbf{f})} \frac{4\pi}{c_{\mathbf{f}}} \mathbf{p}_{\mathbf{f}} e^{\mathbf{f}} - \frac{h^2}{8\pi} \sum_{(\mathbf{f})} \omega_{\mathbf{f}}^2 c_{\mathbf{f}} \frac{\partial^2}{\partial \mathbf{p}_{\mathbf{f}} \partial \mathbf{p}_{\mathbf{f}}}$$

In a number of cases, the ion oscillation frequencies are sufficiently small. Then, the first three terms in the expression for H will be principal and the fourth, corresponding to the kinetic energy of the longitudinal, polarizing ion oscillations, will be small and we obtain, here, a typical example of the coupling we called adiabatic.

Using the introduction of the quantum Bose-amplitudes

$$b_{\mathbf{f}} = \sqrt{\frac{2\pi}{\hbar\omega_{\mathbf{f}}\mathbf{c}_{\mathbf{f}}}} P_{\mathbf{f}} + \sqrt{\frac{\hbar\omega_{\mathbf{f}}\mathbf{c}_{\mathbf{f}}}{8\pi}} \frac{\partial}{\partial P_{-\mathbf{f}}}; b_{\mathbf{f}} = \sqrt{\frac{2\pi}{\hbar\omega_{\mathbf{f}}\mathbf{c}_{\mathbf{f}}}} P_{-\mathbf{f}} - \sqrt{\frac{\hbar\omega_{\mathbf{f}}\mathbf{c}_{\mathbf{f}}}{8\pi}} \frac{\partial}{\partial P_{\mathbf{f}}}$$

the Hamiltonian (2) leads to the general form (1) cited earlier, with the coefficients:

$$2 \int_{\mathbf{f}} = \frac{e}{|\mathbf{f}|} \sqrt{\frac{2\pi h \omega_{\mathbf{f}} c_{\mathbf{f}}}{V}}$$

In order to formulate, mathematically, the assumption on the smallness of the $\omega_{\rm f}$ frequency, we can consider $\sqrt[]{\omega_{\rm f}}$ proportional to some small parameter ϵ . Then $\mathcal{U}_{\rm f}$ is said to be proportional to ϵ and $\hbar\omega_{\rm f}$ to be proportional to ϵ^2 . Consequently, we can speak of adiabatic coupling in the general case of the system described by the Hamiltonian (1), if we put:

(3)
$$2 \int_{\mathbf{f}} = \varepsilon \mathcal{B}_{\mathbf{f}}; \quad h\omega_{\mathbf{f}} = \varepsilon^2 v_{\mathbf{f}}$$

The adiabatic character of the coupling, determined by the Hamiltonian (1) with the coefficients (3), becomes especially explicit if we transform from the Boseamplitudes to the complex coordinates:

(4)
$$q_{f} = \frac{b_{f} + b_{-f}}{\epsilon \sqrt{2}} ; q_{f} = q_{-f}$$

and the canonical conjugate momenta:

(5)
$$-i\frac{\partial}{\partial q_f} = p_f = i\epsilon \frac{b_f - b_{-f}}{\sqrt{2}} ; \quad p_f^{\dagger} = p_{-f}$$

Actually, then the Hamiltonian (1) with the coefficients (3) can be written as:

(6)
$$H = \frac{\stackrel{>}{p}^2}{\stackrel{>}{2}\mu} + \sum_{(\mathbf{f})} A_{\mathbf{f}} q_{\mathbf{f}} e^{i(\stackrel{>}{\mathbf{f}}\mathbf{r})} + \frac{1}{2} \sum_{(\mathbf{f})} v_{\mathbf{f}} q_{-\mathbf{f}} q_{\mathbf{f}} + \frac{\varepsilon^{\frac{1}{4}}}{2} \sum_{(\mathbf{f})} v_{\mathbf{f}} p_{-\mathbf{f}} p_{\mathbf{f}}; \quad A_{\mathbf{f}} = \frac{\mathcal{B}_{\mathbf{f}} + \mathcal{B}_{\mathbf{f}}}{\sqrt{2}}$$

in which the field kinetic energy enters as a small parameter.

Let us note that a number of problems in which the kinetic energy could be considered as a small perturbation was already investigated using perturbation theory.

For example, let us cite the problem of the influence of the nucleus motion on the energy level of the electrons in the molecule [5]. However, the absence of translational degeneration is characteristic for all these solved problems.

In our case of the problem of particle interaction with a field there is always translational degeneration inasmuch as the Hamiltonian (1) is invariant with respect to the group of transformations:

(7)
$$\begin{array}{cccc}
\overrightarrow{r} \rightarrow \overrightarrow{r} + \overrightarrow{a} & ; & \overrightarrow{a} = \text{const} \\
b_f \rightarrow b_f e^{-i(\overrightarrow{fa})} & ; & b_f \rightarrow b_f e^{i(\overrightarrow{fa})}
\end{array}$$

or, in complex coordinates:

(8)
$$\overrightarrow{r} \rightarrow \overrightarrow{r} + \overrightarrow{a} ; q_f \rightarrow q_f e^{-i(\overrightarrow{r}\overrightarrow{a})}$$

Because of the degeneration, the known methods of adiabatic approximation are inapplicable here and it would be necessary to construct a new special form of perturbation theory.

The explanation of this new scheme, developed by the author and S. V. Tiablikov, is the subject of this paper.

Let us make a number of preliminary remarks. Thus, because of the Hamiltonian invariance with respect to the group of transformations (7), the total momentum of the system

$$p + \sum_{(f)} h f b_f b_f = P = const$$

is maintained. Using the variables (4),(5), the total momentum can also be represented as:

(9)
$$P = p - ih \sum_{f} q_{f} p_{f}$$

Since \overrightarrow{P} commutes with \overrightarrow{H} , we can use this vector to enumerate the energy levels. Let us take any independent system of observations ... α_j ... commutating with \overrightarrow{H} which generates a complete system with \overrightarrow{P} and let us denote the energy levels and

the corresponding eigenfunctions through:

$$E = E_{\overrightarrow{P}}, \dots \alpha_{j} \dots ; \qquad \overline{\Psi} = \Psi_{\overrightarrow{P}}, \dots \alpha_{j} \dots$$

Now, let us show that the derivative

is the average particle velocity for the $\Psi_{\tilde{P},\ldots\alpha_{j}}$ state. Actually, let us perform the canonical transformation

in the Hamiltonian (1). Then

$$H = \frac{\left(\frac{1}{2} - h \sum_{f}^{f} \zeta_{f} \zeta_{f}\right)^{2}}{2\mu} + \sum_{f}^{f} \left(\frac{1}{2} + 2 \sum_{f}^{f} \zeta_{f}\right)^{2} + \sum_{f}^{f} h \omega_{f} (\zeta_{f}^{f} \zeta_{f} + \frac{1}{2})$$

and

$$\dot{\hat{r}} = \frac{1}{\mu} (\dot{\hat{P}} - h \sum_{f} \dot{\hat{f}} \dot{\hat{\zeta}}_{f} \dot{\hat{\zeta}}_{f})$$

in which, here, the components of P can be considered as c -numbers.

Let us write the wave equation:

$$(H - \mathbb{E}_{\overrightarrow{P}, \dots \alpha_{j}}) \overline{\Psi}_{\overrightarrow{P}, \dots \alpha_{j}} = 0$$

and let us differentiate it with respect to P. We obtain:

$$(H - E) \frac{\partial \overline{\Psi}}{\partial P} + \left(\frac{\partial \overline{P}}{\partial H} - \frac{\partial \overline{E}}{\partial P}\right) \overline{\Psi} = 0$$

or

$$(H - E) \frac{\partial \Psi}{\partial P} + \left(r - \frac{\partial E}{\partial P}\right)\Psi = 0$$

from which

$$\left(\stackrel{*}{\Psi} \cdot \left(\stackrel{*}{r} - \frac{\partial E}{\partial P} \right) \stackrel{*}{\Psi} \right) = 0$$

that is

$$\frac{\partial \mathbf{E}}{\partial \mathbf{P}} = (\mathbf{\Psi} \cdot \mathbf{r} \mathbf{\Psi})$$

which proves the correctness of the assumption made.

Now, turning to the formulation of the new adiabatic approximation scheme which is applicable to the Hamiltonian of type (6), let us note that it will be more expedient to make certain variable transformations in order to give the wave equation a more convenient form. In order to explain their physical meaning, let us visualize how the particle must move for a state close to the lowest energy level. Evidently, a fluctuating motion - 'tremor' - specified by its interaction with the zero-point oscillations of the field must be imposed on the uniform and rectilinear particle motion.

Let \vec{q} be the part of \vec{r} which refers to the uniform, rectilinear motion and let $\vec{\chi}$ be the fluctuating part.

Keeping in mind the group of transformations (8), it appears natural to us to make the change of variable such that all the variation transforms to \vec{q} , here, reducing (8) to the pure translation \vec{q} without touching upon $\vec{\lambda}$ and the new field coordinates.

Consequently, we should put:

$$\vec{r} = \vec{q} + \vec{\lambda}$$
; $q_f = G_f e^{-i(fq)}$

and should consider (8) as the transformation

for which $\bar{\chi}$ and G_{f} remain invariant. On the other hand, if the parameter ϵ should equal zero exactly, that is, if the field kinetic energy could be neglected completely, the variables G_{f} would commute with the total energy and the energy level could be considered a function of G_{f} :

$$E = E(\ldots G_{e}\ldots)$$

The G would have specific numerical values for the lowest energy level and, precisely those, for which:

$$E(...G_{f}...) = min$$

Because ϵ is small, but not zero, in the case analyzed, we put:

$$G_f = u_f + \varepsilon Q_f$$
; $u_{-f} = u_f$; $Q_{-f} = Q_f$

where $u_{\hat{f}}$ are certain numbers which will be determined later and the $Q_{\hat{f}}$ are new variables. Therefore, we arrive at the change of variable:

(10)
$$\vec{r} = \vec{q} + \vec{\lambda}$$
; $q_f = (u_f + \epsilon Q_f) e^{-i(\vec{q})}$

These transformations introduce instead of the variables $\vec{r}, \dots q_f$... the variables $\vec{q}, \vec{\lambda}, \dots Q_f$... which are three larger in number than before and, consequently, we must impose three independent, additional conditions, for example, on Q_f .

Let us take any complex numbers v_f satisfying the 'substantiality relations' $v_{-f} = \overset{*}{v}_{f}$

and let us impose the three additional conditions

$$\sum_{\mathbf{f}} \mathbf{f} \overset{*}{\mathbf{v}}_{\mathbf{f}} Q_{\mathbf{f}} = 0$$

on $Q_{\hat{\mathbf{f}}}$. In order to simplify the calculations, it will be convenient to choose $\mathbf{v}_{\hat{\mathbf{f}}}$ so that the orthogonality relation

(12)
$$\sum_{(f)} f^{\alpha} f^{\beta} v_{f}^{*} u_{f} = \delta_{\alpha,\beta}$$

where f^{α}, f^{β} are components of the vector f, would be satisfied.

Strictly speaking, these last relations do not limit the freedom of choice of $\mathbf{v}_{\mathbf{f}}$ inasmuch as we can succeed in satisfying (12) for arbitrary $\mathbf{v}_{\mathbf{f}}$ by an appropriate linear transformation in the \mathbf{f} space.

Counting the additional conditions (11), we have just as many independent variables among the new $\vec{q}, \vec{\lambda}, \dots Q_f$... as before.

Now, let us consider the wave equation

$$(H - E)\Psi = 0$$

in which

(13)
$$H = -\frac{h^2}{2\mu} \Delta_r + \sum_{(f)} A_f q_f e^{i(fr)} + \frac{1}{2} \sum_{(f)} v_f q_{-f} q_f - \frac{\epsilon^{l_f}}{2} \sum_{(f)} v_f \frac{\partial}{\partial q_{-f}} \frac{\partial}{\partial q_f}$$

and let us transform it to the new variables by starting from the usual derivative transformation formulas:

$$\frac{\partial}{\partial \mathbf{r}} = \sum_{\mathbf{f}} \frac{\partial Q_{\mathbf{f}}}{\partial \mathbf{r}} \frac{\partial}{\partial Q_{\mathbf{f}}} + \sum_{\mathbf{f}} \frac{\partial Q_{\mathbf{f}}}{\partial \mathbf{r}} \frac{\partial}{\partial \mathbf{r}} + \sum_{\mathbf{f}} \frac{\partial Q_{\mathbf{f}}}{\partial \mathbf{r}} \frac{\partial}{\partial \mathbf{r}} \frac{\partial}{\partial \mathbf{r}} + \sum_{\mathbf{f}} \frac{\partial Q_{\mathbf{f}}}{\partial \mathbf{r}} \frac{\partial}{\partial \mathbf{r$$

First of all, let us note that the relation

$$\sum_{f}^{\Sigma} f v_f^*(q_f e^{i(fq)} - u_f) = 0$$

resulting from (10), (11) shows that \vec{q} is a function of $q_{\vec{f}}$ independent of \vec{r} . Remarking also that

$$Q_{f} = \frac{1}{\varepsilon} (q_{f} e^{i(\hat{f}\hat{Q})} - u_{f})$$

we find from (14)

$$\frac{\partial}{\partial \vec{r}} = \frac{\partial}{\partial \vec{k}}$$
(16)
$$- i \frac{\partial}{\partial q_k} = \frac{1}{\epsilon} e^{i(\vec{k}\vec{q})} P_k^i + \left[\frac{\partial \vec{q}}{\partial q_k} \left(- i \frac{\partial}{\partial q} \right) + i \frac{\partial}{\partial \vec{k}} + i \sum_{(f)} \vec{r} Q_f P_f^i \right]$$

where

$$P_k^{\dagger} = P_k - \tilde{v}_k \sum_{(f)} (kf) u_f P_f$$
; $P_k = -i \frac{\partial}{\partial Q_k}$

In order to clear expression (16) we must find $\frac{\partial \overline{q}}{\partial q_k}$. Hence, let us differentiate (15). We will have:

or

Hence, because of the orthogonality relation (12):

(17)
$$\frac{\partial \vec{q}}{\partial q_k} = i k k k e^{i(kq)} - \epsilon \sum_{(f)} \vec{f} \frac{\partial \vec{q}}{\partial q_k} k f^Q_f = 0$$

Expanding the desired function in a series of powers of the small parameter, we obtain:

$$e^{-(\overrightarrow{kq})} \frac{\partial \overrightarrow{q}}{\partial q_k} = i \overrightarrow{v}_k \left\{ \overrightarrow{k} - \varepsilon \sum_{(f)} \overrightarrow{f} (\overrightarrow{fk}) \overrightarrow{v}_f Q_f + \varepsilon^2 \sum_{(f,g)} \overrightarrow{f} (\overrightarrow{fg}) (\overrightarrow{gk}) \overrightarrow{v}_f \overrightarrow{v}_g Q_f Q_g + \varepsilon^3 \ldots \right\}$$

Substituting these series in (16) and then, together with (10) in (13), we find an explicit expression for the operator H in the new variables represented by an expansion in powers of ε . It is easy to confirm that the variable $\frac{1}{q}$ is not contained explicitly in the transformed operator H, as it should be because of the invariance of H with respect to the translation $q \rightarrow \frac{1}{q} + \frac{1}{\alpha}$.

The variable $\overset{\bullet}{q}$ arises in H only through the canonical momentum conjugate to it.

Let us explain the physical meaning of this quantity.

Because of (10) we have

$$\frac{\partial}{\partial \vec{q}} = \sum_{\{1 \le \alpha \le 3\}} \frac{\partial r^{\alpha}}{\partial \vec{q}} \frac{\partial}{\partial r^{\alpha}} + \sum_{\{f\}} \frac{\partial q_f}{\partial \vec{q}} \frac{\partial}{\partial q_f} = \frac{\partial}{\partial \vec{r}} - i \sum_{\{f\}} \vec{r} q_f \frac{\partial}{\partial q_f}$$

and, consequently,

$$-ih \frac{\partial}{\partial q} = \vec{p} - i \sum_{(f)} h f q_f p_f$$

Therefore, we see on the basis of (9) that the quantity considered is the total momentum of the system:

$$- ih \frac{\partial}{\partial \vec{a}} = \vec{P}$$

Inasmuch as q does not enter explicitly in the transformed operator H, we can

eliminate this variable by putting

$$\bar{\Psi} = \exp\left[\frac{1}{h}(\vec{Pq})\right] F(\vec{\lambda}, ... Q_f...)$$

Then, we obtain the wave equation for F in which $\stackrel{>}{P}$ will enter as the usual c-vector.

It is convenient to introduce instead of \overrightarrow{P} the vector: $\overrightarrow{I} = \varepsilon^{2}\overrightarrow{P}$

As simple computations show, the fact is that if we should consider \overrightarrow{P} to be a 'zero order' quantity, then the dependence of the total energy on \overrightarrow{P} would only appear starting with the fourth approximation in terms of the order of $\varepsilon^{\frac{1}{2}}$.

Considering $\stackrel{\longrightarrow}{P}$ to be a quantity of order $\frac{\stackrel{\longrightarrow}{I}}{\epsilon^2}$ (where $\stackrel{\longrightarrow}{I}$ is a 'zero order' quantity), we will perceive this dependence in the zero approximation.

Finally, let us note that we must still complete one simple tranformation of the wave function

(19)
$$\vec{F} = \exp \left[i \sum_{f} \frac{s_f}{\epsilon} Q_f \right] \phi$$

which reduces to substituting $-i\frac{\partial}{\partial Q}+\frac{s_f}{\epsilon}$ for $-i\frac{\partial}{\partial Q_f}$ in the field energy wave equation, in order to make possible the expansion of the wave function in a series of increasing powers of the small parameter.

Here $\mathbf{s}_{\mathbf{f}}$ are certain complex numbers which we will determine later. Hence, we will require that

in order to guarantee the substantiality of the exponent. Furthermore, since the $Q_{\mathbf{f}}$ variables are related through condition (11), we can put, without limiting the generality of the choice of $s_{\mathbf{f}}$:

$$\begin{array}{ccc} \Sigma & & \\ \Sigma & & \\$$

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Actually, if any s_{f}^{t} do not satisfy these relations, we can always write:

$$s_{f}^{!} = s_{f} + (\overrightarrow{fX}) \overset{*}{v}_{f}$$
; $\overrightarrow{X} = \sum_{(k)} \overrightarrow{k} u_{k} s_{k}^{!}$

and, thus, introduce new quantities s_f which, on the one hand, already satisfy (19_1) and, on the other hand, do not change the value of the exponent under consideration because of (11):

$$\sum_{(f)} s_f^{iQ} f = \sum_{(f)} s_f^{Q} f$$

Carrying out all the transformations mentioned above, we obtain, finally, the wave equation:

(20)
$$(H_0 + \varepsilon H_1 + \varepsilon^2 H_2 + \dots - E)\phi = 0$$

in which

$$H_{0} = -\frac{h^{2}}{2\mu} \Delta_{k} + \sum_{f} A_{f} u_{f} e^{i(\widehat{f}\lambda)} + \frac{1}{2} \sum_{(f)} v_{f} |u_{f}|^{2} + \frac{1}{2} \sum_{(f)} v_{f} |s_{f}| + \frac{i\widehat{v}_{f}}{h} (\widehat{f}f)|^{2}$$

$$H_{1} = \sum_{(f)} v_{f} (\mathring{s}_{f} - \frac{iv_{f}}{h} (\widehat{f}f)) P_{f} f$$

$$+ \sum_{(f)} A_{f} e^{i(\widehat{f}\lambda)} + v_{f} \mathring{u}_{f} - \left(s_{f} + \frac{i\widehat{v}_{f}}{h} (\widehat{f}f)\right) \sum_{(g)} v_{g} (\mathring{s}_{g} - \frac{iv_{g}}{h} (\widehat{f}g)) Q_{g} f$$

$$(21) H_{2} = \frac{1}{2} \sum_{(f)} v_{f} Q_{f} + \frac{1}{2} \sum_{(f)} v_{f} P_{f} + v_{f} \sum_{(g)} (\widehat{f}g) (s_{g} + \frac{i\widehat{v}_{g}}{h} (\widehat{f}g)) Q_{g} f$$

$$P_{f}^{1} - \mathring{v}_{f} \sum_{(g)} (\widehat{f}g) (s_{g} + \frac{i\widehat{v}_{g}}{h} (\widehat{f}g)) Q_{g} f$$

$$+ \sum_{(k,f,g)} v_{k} (\mathring{s}_{k} - \frac{iv_{k}}{h} (\widehat{f}k)) P_{f} (\widehat{f}g) (\widehat{kf}) (s_{g} + \frac{i\widehat{v}_{g}}{h} (\widehat{f}g)) P_{k} (\widehat{f}g) P_{f} f$$

$$- \sum_{(k,f)} v_{k} (\mathring{s}_{k} - \frac{iv_{k}}{h} (\widehat{f}k)) P_{k} (\widehat{k} \cdot \frac{\partial}{\partial \lambda}) - \frac{i}{2} \sum_{(k,j)} v_{k} v_{k} Q_{g} (s_{k} + \frac{i\widehat{v}_{g}}{h} (\widehat{f}k))$$

It should be emphasized that the variables $Q_{\mathbf{f}}$ in these equations are related

through the three relations (11). Since the momenta $P_f = -i \frac{\partial}{\partial Q_f}$ enter into the expression for H only in the combinations

$$P_k^{\dagger} = P_k - \mathring{v}_{k(f)}^{\Sigma} (\mathring{k}f) u_f^{P_f}$$

and since identically

$$P_{\mathbf{k}(\mathbf{f})}^{\mathsf{i}} \stackrel{\Sigma}{f} \stackrel{\mathsf{v}}{\mathbf{v}}_{\mathbf{f}} Q_{\mathbf{f}} - \sum_{\mathbf{f}} \stackrel{\Sigma}{f} \stackrel{\mathsf{v}}{\mathbf{v}}_{\mathbf{f}} Q_{\mathbf{f}} P_{\mathbf{k}}^{\mathsf{i}} = 0$$

then the vector $\sum_{\mathbf{f}} \mathbf{f} \mathbf{v}_{\mathbf{f}}^{\mathbf{Q}}$ commutates with H and (11) are actually compatible with the wave equation (20).

Now, let us apply the usual perturbation theory practices to this equation and let us put:

$$\phi = \phi_0 + \varepsilon \phi_1 + \varepsilon^2 \phi_2 + \dots$$
; $E = E_0 + \varepsilon E_1 + \varepsilon^2 E_2 + \dots$

Then, we obtain:

$$(H_{o} - E_{o})\phi_{o} = 0$$

$$(H_{o} - E_{o})\phi_{1} = -H_{1}\phi_{o} + E_{1}\phi_{o}$$

$$(H_{o} - E_{o})\phi_{2} = -H_{2}\phi_{o} - H_{1}\phi_{1} + E_{2}\phi_{o} + E_{1}\phi_{1}$$

Because of its definition (21), the operator H_0 does not act upon the variables Q_f of the wave function and, consequently, the first of equations (22) has a solution of the form:

$$\phi_{o} = \varphi(\lambda) \theta(\ldots Q_{f} \ldots)$$

with the arbitrary functions $\Theta(\ldots Q_f \ldots)$.

Putting

(23)
$$E_{o} = W + \frac{1}{2} \sum_{(f)} v_{f} |u_{f}|^{2} + \frac{1}{2} \sum_{(f)} v_{f} |s_{f}|^{2} + \frac{i \hat{v}_{f}}{h} (\hat{I}f)|^{2}$$

we see, also, that $\varphi(\overline{\lambda})$ satisfies the equation:

(24)
$$\left(-\frac{h^2}{2\mu} \Delta_{\lambda}^{2} + \sum_{(f)} A_{f} u_{f} e^{i(f\lambda)} - W\right) \Phi(\lambda) = 0$$

Let us assume that the lowest level $W=W_{\rm o}$ for this equation belongs to the discrete spectrum and is separated from the continuous spectrum level by an energy slot.

Let us also assume that the W_0 level for (24) is non-degenerate and let us denote the corresponding normalized eigenfunction through $q_0(\vec{\lambda})$. Then, desiring to investigate the energy level sufficiently close to the lowest level for the system under consideration - particles in a quantum field - we must put in (23):

$$W = W_{O}$$

The appropriate general solution of the first of equations (22) is

$$\phi_{o} = \varphi_{o}(\lambda) \varphi_{o}(\ldots Q_{f}\ldots)$$

with the function Θ_{α} as yet undefined.

Now, let us consider the second of equations (22) and let us note that, identically:

$$\int \overset{*}{\Phi}_{O}(\overset{*}{\lambda})(H_{O} - E_{O})\phi_{1} d\overset{*}{\lambda} = 0$$

Consequently,

(26)
$$\left\{ \int \overset{*}{\varphi}_{o}(\vec{\lambda}) H_{1} \varphi_{o}(\vec{\lambda}) d\vec{\lambda} - E_{1} \right\} \Theta_{o} = 0$$

But the operator

(27)
$$\int \overset{*}{\phi}(\vec{\lambda}) H_1 \varphi_0(\vec{\lambda}) d\vec{\lambda}$$

is a linear form relative to Q_f , P_f^1 and, consequently, (26) cannot have a regular solution with the exception of the case when the operator (27) is identically zero and when, therefore, it is satisfied by the arbitrary function Θ_0 when $E_f = 0$.

Hence, let us select the quantities $u_{\hat{f}}$ and $s_{\hat{f}}$, undefined up till now, so that operator (27) will be annulled.

Here, equating the coefficients with $Q_{\mathbf{f}}$ to zero, we find

(28)
$$A_{\mathbf{f}} \int e^{\mathbf{i}(\widehat{\mathbf{f}}\widehat{\lambda})} |\varphi_{0}(\widehat{\lambda})|^{2} d\widehat{\lambda} + \nu_{\mathbf{f}} \widehat{\mathbf{u}}_{\mathbf{f}} - \left(\mathbf{s}_{\mathbf{f}} + \frac{\mathbf{i}\widehat{\mathbf{v}}_{\mathbf{f}}}{h} \left(\widehat{\mathbf{I}}\widehat{\mathbf{f}}\right)\right) \sum_{(g)} \nu_{g} \left(\mathbf{s}_{g} - \frac{\mathbf{i}\mathbf{v}_{g}}{h} \left(\widehat{\mathbf{I}}\widehat{\mathbf{f}}\right)\right) (\widehat{\mathbf{g}}\widehat{\mathbf{f}}) \widehat{\mathbf{v}}_{g} = 0$$

We cannot, possibly, equate all the coefficients with $P_{\mathbf{f}}^{\mathbf{i}}$ to zero inasmuch as $\mathbf{s}_{\mathbf{f}}^{\mathbf{i}}$ are already related by the three relations (19,), but this is not required.

Actually, because of (21),(28) for the operator (27) to vanish, we must guarantee the equality:

(29)
$$\sum_{(\mathbf{f})} v_{\mathbf{f}} \left(\mathbf{\hat{s}}_{\mathbf{f}} - \frac{i v_{\mathbf{f}}}{h} \right) \mathbf{P}_{\mathbf{f}}^{\dagger} = 0$$

for all possible P_f^1 . But, according to the definition, the P_f^1 satisfy:

$$\sum_{(f)} \mathbf{f} \mathbf{u}_{f} P_{f}^{!} = 0$$

Therefore, (29) will be satisfied if we select s so that

(30)
$$v_{\mathbf{f}}\left(\mathring{\mathbf{s}}_{\mathbf{f}} - \frac{iv_{\mathbf{f}}}{h}\left(\overrightarrow{\mathbf{If}}\right)\right) = -iu_{\mathbf{f}}\left(\overrightarrow{\mathbf{fC}}\right)$$

where \vec{C} is a certain vector which must be defined using (19_1) .

Substituting the value found from (30)

(31)
$$s_{f} = -\frac{i\mathring{v}_{f}}{h} (If) + \frac{i\mathring{u}_{f}}{v_{f}} (Cf)$$

into these relations, we obtain an equation relating \vec{C} to \vec{I} :

(32)
$$\vec{I} = h \sum_{(f)} \vec{f} \frac{(\vec{cf})}{v_f} |u_f|^2$$

Furthermore, substituting the value (30) into (28), we obtain the following expression defining $\mathbf{u}_{\mathbf{r}}$:

(33)
$$u_{f} = -\frac{{\stackrel{*}{A}}_{f}v_{f}}{v_{f}^{2} - (\widetilde{Cf})^{2}} \int e^{-i(\widetilde{f}\lambda)} |\phi_{o}(\lambda)|^{2} d\lambda$$

The formulas (31), (32), (33) which are found enable s_f , u_f to be determined if $\Phi_o(\lambda)$ be known.

In order to determine this latter, we would have (24) which now can be written:

$$\left(-\frac{h^2}{2\mu}\Delta_{\lambda}^{2} + U(\lambda) - W_0\right)\phi_0(\lambda) = 0$$

(35)
$$U(\lambda) = -\sum_{(f)} \frac{v_f |A_f|^2 f e^{-i(f\lambda)} |\phi_o(\lambda)|^2 d\lambda}{v_f^2 - (Cf)^2} e^{i(f\lambda)}$$

Let us note that since it is required that W_0 be non-degenerate for the theory explained to be applicable, we can always consider the real eigenfunction $\Phi(\lambda)$. It is expedient to use its extremal property

(36)
$$I(\varphi) = \frac{h^2}{\mu} \int \left(\frac{\partial \varphi}{\partial \lambda}\right)^2 d\lambda - \sum_{(\mathbf{f})} \frac{\nu_{\mathbf{f}} |A_{\mathbf{f}}|^2}{\nu_{\mathbf{f}}^2 - (\hat{C}_{\mathbf{f}})^2} \Big| \int e^{-i(\hat{f}\lambda)} \varphi^2(\lambda) d\lambda \Big|^2 = \min$$

with the condition

in order to determine it in fact.

Before proceeding to the discussion of the properties of the first approximation obtained, let us continue the analysis of the second of equations (22) and let us note that, on the basis of the above, this equation can be represented as:

$$\left(-\frac{h^2}{2\mu}\Delta_{\lambda}^2 + U(\lambda) - W\right)\phi_1 = -(H_1 - \int \dot{\phi}_0(\lambda)H_1\phi_0(\lambda) d\lambda)\phi_0(\lambda)\phi_0(\ldots\phi_f\ldots)$$

In order to find ϕ_1 let us consider the eigenfunctions $\phi_n(\vec{\lambda})$ (n \neq 0) of the equation:

(38)
$$\left(-\frac{h^2}{2\mu} \Delta_{\lambda}^{2} + U(\lambda) - W_{n}\right) \varphi_{n}(\lambda) = 0$$

which generate with $\varphi_{o}(\tilde{\lambda})$ a complete orthonormal system of eigenfunctions.

Then, evidently:

(39)
$$\phi_{1} = -\sum_{(n \neq 0)} \varphi_{n}(\overline{\lambda}) \frac{\int_{n}^{\varphi_{n}}(\overline{\lambda}) H_{1} \varphi_{0}(\overline{\lambda}) d\overline{\lambda}}{W_{n} - W_{0}} \Theta_{0}(\dots Q_{f}\dots) + \varphi_{0}(\overline{\lambda}) \Theta_{1}(\dots Q_{f}\dots)$$

where $\theta_1(\ldots Q_f\ldots)$ is as yet an arbitrary function. Evidently, the summation here also includes the integration over the continuous spectrum.

Now, let us consider the third of equations (22) and let us write it as:

$$\left(-\frac{h^2}{2\mu}\Delta_{\lambda}^{+} + U(\lambda) - W_0\right)\phi_2 = -H_2\phi_0\theta_0 + E_2\phi_0\theta_0 - H_1\phi_1$$

The condition that this equation be solvable is:

$$\int \overset{*}{\varphi}_{0}(\vec{\lambda}) H_{2} \varphi_{0}(\vec{\lambda}) \theta_{0} d\vec{\lambda} + \int \overset{*}{\varphi}_{0}(\vec{\lambda}) H_{1} \phi_{1} d\vec{\lambda} - E_{2} \theta_{0} = 0$$

or taking (39) into account

$$(\Gamma - \mathbb{E}_{2}) \Theta_{0}(\dots Q_{1}\dots) = 0$$

$$(40) \qquad \Gamma = \int_{0}^{\frac{\pi}{\varphi_{0}}} (\lambda) H_{2} \Psi_{0}(\lambda) d\lambda - \sum_{(n \neq 0)} \frac{\int_{0}^{\frac{\pi}{\varphi_{0}}} (\lambda) H_{1} \Psi_{n}(\lambda) d\lambda}{W_{n} - W_{0}} \frac{\lambda}{W_{n} - W_{0}} (\lambda) d\lambda$$

Therefore, the solvability condition of the second approximation equation leads to an equation determining θ_0 , E_2 . Similarly, the solvability condition of the third approximation equation yields an equation determining θ_1 , E_3 etc.

Now, having explained the process of successively obtaining the coefficients of our power expansion, let us turn to the analysis of the first approximation.

Since $E_1 = 0$, then the energy of the system will be, according to (23) (30), in this approximation:

(41)
$$E_{o} = W_{o} + \frac{1}{2} \sum_{(f)} |u_{f}|^{2} \left(v_{f} + \frac{(fc)^{2}}{v_{f}}\right)$$

Hence, differentiating we find:

$$(42) \qquad \frac{\partial E_o}{\partial c^{\alpha}} = \frac{\partial W_o}{\partial c^{\alpha}} + \frac{1}{2} \sum_{(f)} \left(\frac{\partial \tilde{u}_f}{\partial c^{\alpha}} u_f + \tilde{u}_f \frac{\partial u_f}{\partial c^{\alpha}} \right) \left(v_f + \frac{(fc)^2}{v_f} \right) + \sum_{(f)} f^{\alpha} \frac{|u_f|^2}{v}$$

On the other hand, differentiating (24), we obtain:

$$\left\{ -\frac{h^2}{2\mu} \Delta_{\lambda}^{+} + \sum_{(f)}^{\Sigma} A_f u_f e^{i(f\lambda)} - W_o \right\} \frac{\partial \varphi_o(\lambda)}{\partial c^{\alpha}} + \sum_{(f)}^{\Sigma} A_f \frac{\partial u_f}{\partial c^{\alpha}} e^{i(f\lambda)} \varphi_o(\lambda) - \frac{\partial W_o}{\partial c^{\alpha}} \varphi_o(\lambda) = 0$$

from which

$$\frac{\partial W_{o}}{\partial C^{\alpha}} = \sum_{(f)}^{\Sigma} A_{f} \int e^{i(f\lambda)} |\phi_{o}(\lambda)|^{2} d\lambda \frac{\partial u_{f}}{\partial C^{\alpha}} = -\sum_{(f)}^{\Sigma} \left(v_{f} - \frac{(fC)^{2}}{v_{f}}\right) \mathring{u}_{f}^{*} \frac{\partial u_{f}}{\partial C^{\alpha}}$$

and, consequently, on the basis of (42) and (32):

$$\frac{\partial \hat{z}_{0}}{\partial c^{\alpha}} = -\sum_{(\mathbf{f})} \left(v_{\mathbf{f}} - \frac{(\mathbf{f}_{0})^{2}}{v_{\mathbf{f}}} \right) \mathring{\mathbf{u}}_{\mathbf{f}} \frac{\partial \mathbf{u}_{\mathbf{f}}}{\partial c^{\alpha}} + \frac{1}{2} \sum_{(\mathbf{f})} \left(\frac{\partial \mathring{\mathbf{u}}_{\mathbf{f}}}{\partial c^{\alpha}} \right) \mathbf{u}_{\mathbf{f}} + \frac{\mathring{\mathbf{u}}_{\mathbf{f}}}{\partial c^{\alpha}} \left(\frac{\partial \mathbf{u}_{\mathbf{f}}}{\partial c^{\alpha}} \right) \mathbf{u}_{\mathbf{f}} + \frac{\mathcal{L}_{\mathbf{f}_{0}}}{\partial c^{\alpha}} \left(\frac{\partial \mathbf{u}_{\mathbf{f}}}{\partial c^{\alpha}} \right) \mathbf{u}_{\mathbf{f}} + \frac{\mathcal{L}_{\mathbf{f}_{0}}}{\partial c^{\alpha}} \mathbf{u}_{\mathbf{f}} + \frac{\mathcal{L}_{\mathbf{f}_{0}}}{\partial c^{$$

Therefore, we have:

$$\frac{\partial \mathcal{E}_{0}}{\partial I^{\alpha}} = \sum_{(1 \leq \gamma \leq 3)} \frac{\partial \mathcal{E}_{0}}{\partial C^{\gamma}} \frac{\partial C^{\gamma}}{\partial I^{\alpha}} = \frac{1}{h} \sum_{(1 \leq \beta \leq 3)} C^{\beta} \left\{ \sum_{(1 \leq \gamma \leq 3)} \frac{\partial I^{\beta}}{\partial C^{\gamma}} \frac{\partial C^{\gamma}}{\partial I^{\alpha}} \right\} = \frac{1}{h} \sum_{(1 \leq \beta \leq 3)} C^{\beta} \frac{\partial I^{\beta}}{\partial I^{\alpha}} = \frac{1}{h} C^{\alpha}$$

that is

$$\overrightarrow{C} = h \frac{\partial \mathcal{E}_0}{\partial I} = \frac{h}{\epsilon^2} \frac{\partial \mathcal{E}_0}{\partial P}$$

But \mathcal{E}_{o} is the system energy in the approximation assumed and, consequently,

$$\frac{\partial \mathcal{E}_{0}}{\partial P} = \vec{v}_{av}$$

where v_{av} is the average particle velocity. Therefore, we see that the vector v_{av} represents this average velocity to the accuracy of the factor $\frac{h}{\epsilon^2}$.

Now we can turn to the determination of the particle effective mass.

Let us denote the value of $\Psi_0(\lambda)$, W_0 for C=0 through $\Psi_0(\lambda)$, W_0 , W_0 . We have:

$$\left(-\frac{h^2}{2\mu} \Delta_{\lambda}^2 + U_o(\lambda) - W_{o,o} \right)^{\varphi}_{o,o}(\lambda) = 0$$

$$U_o(\lambda) = -\sum_{(f)} \frac{|A_f|^2}{v_f} \int e^{-i(f\lambda)} |\psi_{o,o}(\lambda)|^2 d\lambda$$

For simplicity, let us assume that $|A_f|^2$, v_f are radially symmetric functions of the quasi-wave vector \overrightarrow{f} and that $\varphi_{0,0}(\overrightarrow{\lambda})$ is radially symmetric relative to $\overrightarrow{\lambda}$. Then, expanding E_0 in powers of C, we obtain if we stop at the term proportional to C^2 :

(44)
$$E_{o} = E_{o,o} + \frac{1}{6} \sum_{f} \frac{hf^{2}}{v_{f}} |u_{f}^{(o)}|^{2} c^{2}$$

where

$$E_{o,o} = W_{o,o} + \frac{1}{2} \sum_{(f)} v_f |u_f^{(o)}|^2$$

$$u_f^{(o)} = -\frac{A_f^*}{v_f} / e^{-i(f\lambda)} |\phi_{o,o}(\lambda)| d\lambda$$

or

$$E_o = E_{o,o} + \frac{v_{av}^2}{2} \sum_{(f)} \frac{h^2 f^2}{3v_f \epsilon^4} |u_f^{(o)}|^2$$

Therefore, the effective mass in the first approximation will be:

$$\mu_{\text{eff}} = \frac{1}{3} \sum_{\text{(f)}} \frac{h^2 f^2}{3 v_f \epsilon^4} |u_f^{(o)}|^2$$

Let us note that (43), for the case cited earlier of electron motion in an ionic crystal, in the form of an appropriate variational principle and (44) for the energy were obtained first by S. I. Pekar [6] using semiclassical theory in which the electron is considered quantum and the field, classical. Starting from the same semiclassical theory, L. D. Landau and S. I. Pekar [7] first obtained a formula for the effective mass.

Here, still within the limits of the first approximation, we can find a correction to (44) showing the deviation of the dependence of the energy and velocity on the quadratic.

In order to do this, it is sufficient to determine $\Psi_0(\vec{\lambda}), W_0$ from (34), (35) to the accuracy of terms of order C^2 inclusively.

Substituting the expansions in powers of C:

$$\varphi_{o}(\overline{\lambda}) = \varphi_{o,o}(\overline{\lambda}) + \sum_{(\alpha,\beta)} C^{\alpha}C^{\beta} \Psi_{\alpha,\beta}(\overline{\lambda}) + \dots$$

$$W_{o} = W_{o,o} + \sum_{(\alpha,\beta)} C^{\alpha}C^{\beta}S_{\alpha,\beta} + \dots$$

in these equations, we obtain the linear equation determining $\Psi_{\alpha,\beta}$, $S_{\alpha,\beta}$:

$$\begin{split} \left\{ -\frac{h^{2}}{2\mu} \Delta_{\lambda}^{2} + U_{o}(\vec{\lambda}) - W_{o,o} \right\} \Psi_{\alpha,\beta}(\vec{\lambda}) - 2 \sum_{(\mathbf{f})} \frac{|A_{\mathbf{f}}|^{2}}{v_{\mathbf{f}}} e^{\mathbf{i}(\mathbf{f}\lambda)} \int e^{-\mathbf{i}(\mathbf{f}\lambda)} \phi_{o}(\vec{\lambda}) \Psi_{\alpha,\beta}(\vec{\lambda}) d\vec{\lambda} = \\ &= \left\{ \sum_{(\mathbf{f})} \frac{|A_{\mathbf{f}}|^{2}}{v_{\mathbf{f}}^{2}} f^{\alpha} f^{\beta} e^{\mathbf{i}(\mathbf{f}\lambda)} \int e^{-\mathbf{i}(\mathbf{f}\lambda)} |\phi_{o}(\vec{\lambda})|^{2} d\vec{\lambda} + S_{\alpha,\beta} \right\} \phi_{o}(\vec{\lambda}) \end{split}$$

Moreover, because of the normalization condition, we have:

$$\int \Psi_{\alpha,\beta}(\vec{\lambda}) \Psi_{0}(\vec{\lambda}) \ \vec{d} \vec{\lambda} = 0$$

It is easy to note that in the case considered:

$$\Psi_{\alpha,\beta}(\vec{\lambda}) = \lambda^{\alpha} \lambda^{\beta} \ \forall (|\vec{\lambda}|) ; S_{\alpha,\beta} = W_{0,1} \delta_{\alpha,\beta}$$

Consequently, in the appropriate expansions

$$u_{f} = u_{f}^{(o)} + \sum_{(\alpha,\beta)} C^{\alpha}C^{\beta} u_{f}^{(\alpha,\beta)} + \dots$$

$$u_{f}^{(\alpha,\beta)} = \frac{f^{\alpha}f^{\beta}}{v_{f}^{2}} u_{f}^{(o)} - 2 \frac{A_{f}^{*}}{v_{f}} \int e^{-i(\widehat{f}\lambda)} \varphi_{o}(\widehat{\lambda}) \lambda^{\alpha} \lambda^{\beta} \Psi(|\widehat{\lambda}|) d\widehat{\lambda}$$

we can write:

$$u_f^{(\alpha,\beta)} = A_f^* f^{\alpha} f^{\beta} \rho_1(|f|)$$

where $\rho_1(|\vec{f}|)$ is the real radially symmetric function of the quasi-wave vector. Obviously, we also have:

$$u_f^{(o)} = A_f^* \rho_o(|\vec{f}|)$$

where $\rho_0(|\vec{f}|)$ is a real radially symmetric function of \vec{f} .

Therefore, substituting the expansion (45) into (32), we find:

$$\vec{I} = \frac{h}{3} \sum_{(f)} \frac{f^2}{v_f} |A_f|^2 \rho_0^2 (|\vec{f}|) \vec{c} + \frac{lih}{5} \sum_{(f)} \frac{f^{l_f} c^2}{v_f} |A_f|^2 \rho_0 (|\vec{f}|) \rho_1 (|\vec{f}|) \vec{c}$$

from which

(46)
$$E_{o} = E_{o,o} + \frac{c^{2}}{6} \sum_{(f)}^{\Sigma} \frac{f^{2}}{v} |A_{f}|^{2} |P_{o}^{2}(|f|) + \frac{3c^{4}}{5} \sum_{(f)}^{\Sigma} \frac{f^{4} |A_{f}|^{2}}{v_{f}} |P_{o}(|f|) |P_{f}(|f|)$$

Therefore, we can give an estimate for the limits of applicability of the square law of the dependence of the energy on the particle velocity.

Now, let us turn to the second approximation equation, (40).

Exposing it using (21) we obtain:

where

$$E' = E_2 - i \int \overset{*}{\phi}_{0}(\vec{\lambda}) \left(\vec{c} \frac{\partial}{\partial \vec{\lambda}}\right) \phi_{0}(\vec{\lambda}) d\vec{\lambda}$$

$$2I_{f,g} = -2A_f^*A_{g(n\neq 0)} \frac{\int_{0}^{*} \phi(\lambda) e^{-i(f\lambda)} \phi(\lambda) d\lambda}{W_n - W_0} \int_{0}^{*} \phi(\lambda) e^{i(g\lambda)} \phi(\lambda) d\lambda$$

and

$$(49) \qquad P_{\mathbf{f}}^{!} = P_{\mathbf{f}}^{!} - i \overset{*}{\mathbf{v}}_{\mathbf{f}} \frac{(\overrightarrow{\mathsf{Cg}})(\overrightarrow{\mathsf{gf}})}{v_{\mathbf{g}}} \overset{*}{\mathbf{u}}_{\mathbf{f}}^{\mathsf{Q}}_{\mathbf{g}} = P_{\mathbf{f}} - \overset{*}{\mathbf{v}}_{\mathbf{f}} \overset{\Sigma}{(\mathbf{gf})} \underbrace{(\overrightarrow{\mathsf{gf}})}_{\mathbf{g}} \underbrace{u_{\mathbf{g}}^{\mathsf{P}}}_{\mathbf{g}} - i \overset{*}{\mathbf{v}}_{\mathbf{f}} \overset{\Sigma}{(\mathbf{gf})} \underbrace{(\overrightarrow{\mathsf{Cg}})(\overrightarrow{\mathsf{gf}})}_{\mathbf{v}_{\mathbf{g}}} \overset{*}{\mathbf{u}}_{\mathbf{g}}^{\mathsf{Q}}_{\mathbf{g}}$$

As is seen, the problem of solving (47) leads to the diagonalization of a quadratic form. Let us note that the sign of this form is related to the properties of the minimum in the variational problem (36),(37).

Thus, it is easy to show that if $\varphi_0(\lambda)$ really realizes the minimum and if, therefore, the appropriate second variation would be positive, then the quadratic form under consideration, Ω , will be positive. This second variation always vanishes for a variation of the form (the solutions of the appropriate Jacobi equation):

$$\delta \Phi = \left(\frac{\partial \Phi_{0}(\lambda)}{\partial \lambda} \cdot \delta \vec{x} \right)$$

with the arbitrary constant $\delta \vec{x}$ inasmuch as the integrals (36),(37) do not vary when $\phi(\vec{\lambda})$ is replaced by $\phi(\vec{\lambda} + \vec{\lambda})$.

Now, if the second variation is essentially positive for any $\delta \phi$ then it can be shown that the quadratic form, Ω , will be positive definite and will become zero only when, identically:

...
$$Q_{f} = 0$$
...; ... $P_{f}^{1} = 0$...

In this case, the positive definiteness of the analyzed quadratic form is diagonalized by means of the canonical transformation:

(50)
$$Q_{\mathbf{f}} = \frac{1}{\sqrt{2}} \sum_{(\omega)} \left\{ \bar{\Psi}_{\omega}(\mathbf{f}) \stackrel{+}{b}_{\omega} + \stackrel{*}{\Psi}_{\omega}(-\mathbf{f}) \stackrel{+}{b}_{\omega} \right\}$$

$$P_{\mathbf{f}}^{\dagger} = \frac{1}{\sqrt{2}} \sum_{(\omega)} \left\{ X_{\omega}(-\mathbf{f}) \stackrel{+}{b}_{\omega} - \stackrel{*}{X}_{\omega}(\mathbf{f}) \stackrel{+}{b}_{\omega} \right\}$$

introducing in place of the complex coordinates and the momenta, related through

to the usual quantum Bose-amplitudes b_{ω} , b_{ω} .

In this approximation, $\Psi_{\omega}(f)$, $X_{\omega}(f)$ represent a system of "eigenfunctions" determined through the equations:

$$\begin{split} & \boldsymbol{\xi}_{\omega} \boldsymbol{\Psi}_{\omega}(\mathbf{f}) = \boldsymbol{\nu}_{\mathbf{f}} \boldsymbol{\tilde{\chi}}_{\omega}(\mathbf{f}) - \boldsymbol{u}_{\mathbf{f}_{(g)}} \boldsymbol{\tilde{\chi}}_{\mathbf{g}} \boldsymbol{\tilde{\chi}}_{\mathbf{g}} \boldsymbol{\tilde{\chi}}_{\omega}(\mathbf{g}) + (\overrightarrow{\mathbf{cf}}) \boldsymbol{\Psi}_{\omega}(\mathbf{f}) - \boldsymbol{u}_{\mathbf{f}_{(g)}} \boldsymbol{\tilde{\chi}}_{\mathbf{g}} \boldsymbol{\tilde{\chi}}_{\mathbf{g}} \boldsymbol{\tilde{\chi}}_{\mathbf{g}} \boldsymbol{\tilde{\chi}}_{\omega}(\mathbf{g}) \\ & \boldsymbol{\tilde{\xi}}_{\omega} \boldsymbol{\chi}_{\omega}(\mathbf{f}) = \boldsymbol{\nu}_{\mathbf{f}} \boldsymbol{\Psi}_{\omega}(\mathbf{f}) + \boldsymbol{\Sigma}_{(g)} \boldsymbol{\mathcal{Y}}_{\mathbf{f}_{\mathbf{g}}} \boldsymbol{\tilde{\chi}}_{\omega}(\mathbf{g}) - \boldsymbol{v}_{\mathbf{f}_{(g)}} \boldsymbol{\tilde{\chi}}_{\mathbf{g}} \boldsymbol{\tilde{\chi}}$$

where

(52)
$$\widetilde{X}_{\omega}(f) = X_{\omega}(f) + v_{f} \sum_{(g)} \frac{(fg)(gC)}{v_{g}} \overset{*}{u}_{g} \psi_{\omega}(g)$$

and the orthonormalization conditions in accordance with it:

(53)
$$\sum_{(\mathbf{f})} \tilde{\mathbf{f}} \overset{*}{\nabla}_{\mathbf{f}} \Psi_{\omega}(\mathbf{f}) = 0 \quad ; \quad \sum_{(\mathbf{f})} \tilde{\mathbf{f}} \overset{*}{u}_{\mathbf{f}} X_{\omega}(\mathbf{f}) = 0$$

$$\sum_{(\mathbf{f})} \left\{ \Psi_{\omega_{1}}(\mathbf{f}) \overset{*}{\nabla}_{\omega_{2}}(\mathbf{f}) + \overset{*}{\Psi}_{\omega_{2}}(\mathbf{f}) X_{\omega_{1}} \right\} = 2\delta(\omega_{1} - \omega_{2})$$

$$\sum_{(\mathbf{f})} \left\{ \Psi_{\omega_{1}}(-\mathbf{f}) X_{\omega_{2}}(\mathbf{f}) - \Psi_{\omega_{2}}(\mathbf{f}) X_{\omega_{1}}(-\mathbf{f}) \right\} = 0$$

The corresponding eigenvalues $\overline{\mathcal{E}}_{\omega}$ are all positive in the case considered. Carrying out the canonical transformation in (47), we obtain:

(54)
$$\left\{\sum_{(\omega)} \mathbf{E}_{\omega} \left(n_{\omega} + \frac{1}{2} \right) - \mathbf{E} \right\} \Theta_{0} = 0 \quad ; \quad n_{\omega} = \overset{*}{b}_{\omega} b_{\omega}$$

which has an obvious solution.

Therefore, the second approximation energy of the system will be:

(55)
$$E = W_o + \frac{1}{2} \sum_{(\mathbf{f})} |\mathbf{u}_{\mathbf{f}}|^2 \left(v_{\mathbf{f}} + \frac{(\mathbf{c}\mathbf{f})^2}{v_{\mathbf{f}}} \right) + \varepsilon^2 \int_{0}^{\infty} (\mathbf{x}) \left(\vec{c} \cdot \mathbf{i} \frac{\partial}{\partial \mathbf{x}} \right) v_{\mathbf{o}}(\mathbf{x}) d\mathbf{x} + \varepsilon^2 \sum_{(\omega)} \mathbf{E}_{\omega} \left(\mathbf{n}_{\omega} + \frac{1}{2} \right)$$

and, in particular, for our energy level:

$$E = W_{o} + \frac{1}{2} \sum_{(\mathbf{f})} |\mathbf{u}_{\mathbf{f}}|^{2} \left(v_{\mathbf{f}} + \frac{(\mathbf{\widetilde{C}f})^{2}}{v_{\mathbf{f}}} \right) + \varepsilon^{2} \int_{0}^{\infty} (\vec{\lambda}) \left(\vec{C} \cdot \mathbf{i} \frac{\partial}{\partial \vec{\lambda}} \right) \phi_{o}(\vec{\lambda}) d\vec{\lambda} + \frac{\varepsilon^{2}}{2} \sum_{(\omega)} \vec{\xi}_{\omega}$$

On the other hand, the energy of a pure field at absolute zero temperature when there are no particles equals:

$$\frac{1}{2} \sum_{(k)}^{\sum} h \omega_k = \frac{\varepsilon^2}{2} \sum_{(k)}^{\sum} \nu_k$$

Consequently, we must take as the energy of particles in a field at absolute zero:

(56)
$$E_{p} = W_{o} + \frac{1}{2} \sum_{(\mathbf{f})} |\mathbf{u}_{\mathbf{f}}|^{2} \left(v_{\mathbf{f}} + \frac{(\mathbf{c}_{\mathbf{f}})^{2}}{v_{\mathbf{f}}} \right) + \varepsilon^{2} \int_{0}^{*} (\mathbf{\lambda}) \left(\mathbf{c} \cdot \mathbf{i} \frac{\partial}{\partial \mathbf{\lambda}} \right) \phi_{o}(\mathbf{\lambda}) d\mathbf{\lambda}$$

$$+ \frac{\varepsilon^{2}}{2} \sum_{(\omega)} (\mathbf{c}_{\omega} - v_{\omega})$$

Expanding this expression in a power series in the velocity

(57)
$$E_{p} = E_{p}^{o} + \frac{\mu_{eff}}{2} v_{av}^{2}$$

we obtain a correction of order ϵ^2 to E_p^o , the energy binding the particles to the field and to the effective mass.

In the general case, expanding (55) in powers of v_{av} (with the exception of the energy of the pure field), it is easy to note that the corresponding corrections will depend on the temperature.

In fact, completing the computation is made more difficult by the complexity of determining the eigenvalues from the system (51).

However, in substance, it is not necessary for us to be able to evaluate the individual $\vec{\epsilon}_{\alpha}$.

It is sufficient to have a method of determining a sum of the type:

$$\sum_{(\omega)} \left\{ \bar{\mathcal{E}}_{\omega}^{} \bar{\mathcal{F}}(\bar{\mathcal{E}}_{\omega}) - \nu_{\omega}^{} \mathcal{F}(\nu_{\omega}) \right\}$$

Since these sums are symmetric functions of $\vec{\delta}_{\omega}$, a method to calculate them directly according to the given coefficients of (51) can be developed without relying on finding the individual $\vec{\delta}_{\omega}$.

An explanation of such a method is the subject of the next paper.

In conclusion, let us note that the development of the above first approximation theory is not altered if we take, not the minimum in (24), but any other discrete spectrum (as long as it is not degenerate).

Therefore, we investigated the possible excited states of particles in a field.

The transformation to the second approximation shows that these states are quasi-stationary and have finite life time.

The case of degenerate states requires special analysis and certain improvement of the substitution of variables (10).

March, 1950

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Mr. Theodore D. Schultz of MIT has called my attention to certain inadequacies and inaccuracies in my translation of the Bogoliubov paper which are due, equally, to my misinterpretation and to the poor quality of Russian printing.

First, since the European notation is used, the following corrections should be made throughout:

$$(\overrightarrow{f} \overrightarrow{r}) \longrightarrow (\overrightarrow{f} \cdot \overrightarrow{r})$$
$$[\overrightarrow{f} \overrightarrow{r}] \longrightarrow (\overrightarrow{f} x \overrightarrow{r})$$
$$(f \cdot r) \longrightarrow (f, r)$$

A list of other corrections follows:

Page	Line	
ı	13 from bottom	nonperiodic should read periodic
6	2 from bottom	observations should read observables
8	12 from bottom	all the variation should read: the whole variation translates on \vec{q} .
9	13 from bottom	substantiality should read reality
10	10 from top	should read (15)
10	3 from bottom	clear should read clarify
10	6 from bottom	last term in (16) should read
		$\frac{\partial \vec{q}}{\partial q_k} - i \frac{\partial}{\partial \vec{q}} + i \frac{\partial}{\partial \vec{\lambda}} + i \sum_{(f)} \vec{f} Q_f P_f$
12	4 from bottom	substantiality should read reality
15	3 from top	slot should read gap
15	5 from top	$q_o(\lambda)$ should read $\Phi_o(\lambda)$
16	l from top	with P' should read of P' f
16	4 from bottom	Paragraph should read: The formulas (31)(32),(33) found
21	3 from bottom	Exposing should read expanding or developing
22	2 from bottom	Paragraph should start: In this case of positive
		definiteness, the analyzed quadratic form etc.